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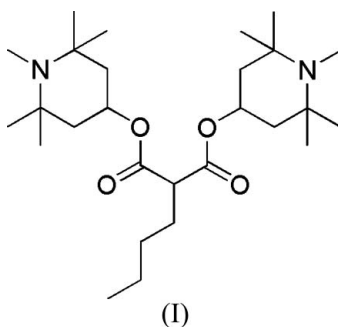
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## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.054  
 $wR$  factor = 0.165  
Data-to-parameter ratio = 16.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(1,2,2,6,6-pentamethylpiperidin-4-yl)  
butylmalonateThe title compound,  $\text{C}_{27}\text{H}_{50}\text{N}_2\text{O}_4$ , was prepared from butylmalonic acid and 1,2,2,6,6-pentamethyl-4-hydroxypiperidine by transesterification. In the molecule, both piperidine rings adopt chair conformations.Received 5 June 2006  
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## Comment

Tinuvin 144 is a light stabilizer of the hindered amine class that also contains an antioxidant unit of the sterically hindered phenol type. Its efficiency provides significantly extended lifetime to coatings by minimizing paint defects such as cracking and loss of gloss (Rasberger, 1980). The title compound, (I), is a key intermediate in the preparation of Tinuvin 144 and was prepared from butylmalonic acid and 1,2,2,6,6-pentamethyl-4-hydroxypiperidine by transesterification using tetraisopropyl orthotitanate as catalyst (Rody, 1983). Selected bond length and angles of (I) are shown in Table 1. Both piperidine rings adopt chair conformations.



## Experimental

A mixture of butylmalonic acid (9.4 g, 0.05 mol), 1,2,2,6,6-pentamethyl-4-hydroxypiperidine (18.8 g, 0.11 mol) and toluene (100 ml) was heated to reflux. Tetraisopropyl orthotitanate (0.2 g) was added and the mixture stirred for 8 h. The reaction mixture was diluted with toluene (200 ml), extracted with water (100 ml) each time, and then dried and concentrated by evaporation. Suitable crystals of the title compound (yield 21.6 g, 92.7%; m.p. 328–329 K) were obtained by slow evaporation of a solution of (I) in a mixture of toluene and cyclohexane (1:2 *v/v*).

## Crystal data

 $\text{C}_{27}\text{H}_{50}\text{N}_2\text{O}_4$   
 $M_r = 466.69$   
Monoclinic,  $P2_1/c$   
 $a = 11.871$  (3) Å  
 $b = 18.170$  (4) Å  
 $c = 13.260$  (3) Å  
 $\beta = 91.386$  (4)°  
 $V = 2859.4$  (11) Å<sup>3</sup> $Z = 4$   
 $D_x = 1.084$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
Block, colourless  
 $0.22 \times 0.20 \times 0.10$  mm

*Data collection*

Bruker SMART-CCD area-detector diffractometer	14581 measured reflections
$\varphi$ and $\omega$ scans	5037 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2237 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.984$ , $T_{\max} = 0.993$	$R_{\text{int}} = 0.066$
	$\theta_{\max} = 25.0^\circ$

*Refinement*

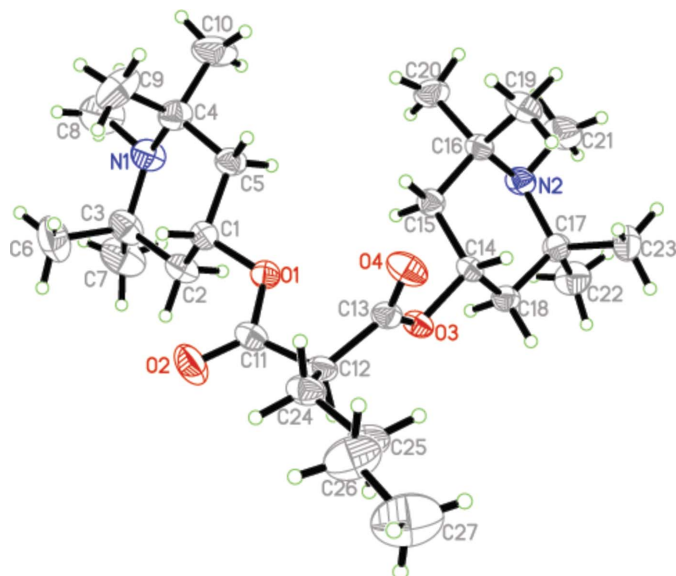
Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.2574P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.165$	$(\Delta/\sigma)_{\max} = 0.002$
$S = 1.02$	$\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$
5037 reflections	$\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$
309 parameters	
H-atom parameters constrained	

**Table 1**Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C11	1.329 (3)	O2—C11	1.199 (3)
O1—C1	1.465 (3)	N1—C8	1.466 (4)
C11—O1—C1	117.8 (2)	O2—C11—C12	123.3 (3)
C8—N1—C3	113.7 (3)	O1—C11—C12	112.4 (3)
C3—N1—C4	119.7 (2)	C11—C12—C13	110.9 (2)
O1—C1—C5	105.8 (2)		
C11—O1—C1—C5	160.6 (2)	O2—C11—C12—C24	−48.8 (4)
O1—C1—C2—C3	−175.8 (2)	O2—C11—C12—C13	−172.4 (3)
C1—O1—C11—O2	5.9 (4)		

The terminal C atoms of the butyl chain, namely C26 and C27, have larger than normal anisotropic displacement parameters and may be slightly disordered. There is no significant residual electron density in the vicinity of these atoms after anisotropic refinement, and the current structure model was therefore found to be acceptable. All H atoms were positioned geometrically and refined using a riding-model approximation ( $\text{C—H} = 0.96\text{--}0.98 \text{ \AA}$ ), with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve

**Figure 1**

A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

**References**

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